CLAIMS

1. A crystallization parameter optimization process comprising the steps of:

selecting a plurality of physical characterization input variables to define a total crystallization experiment permutation number for a crystallant;

performing a plurality of crystallization experimental samples, said plurality of crystallization experimental samples being less than the total crystallization experiment permutation number;

training a predictive crystallization function through analysis of said plurality of crystallization experimental samples; and

determining an optimal physical crystallization parameter from said predictive crystallization function.

2. The process of claim 1 wherein said predictive crystallization function is a neural network.

3. The process of claim 1 wherein said crystallant is a protein.

4. The process of claim 1 wherein each of said plurality of physical crystallization input variables is selected from a group consisting of: temperature, protein dilution, anionic precipitate, organic precipitate, buffer pH, precipitation strength, organic moment, percent glycerol, additive, divalent ion, gravity, light, magnetism, atmosphere identity, and atmosphere pressure.

5. The process of claim 1 wherein the plurality of crystallization experimental samples performed is less than 5% of the total crystallization experiment permutation number.

6. The process of claim 1 wherein the plurality of crystallization experimental samples performed is less than 0.1% of the total crystallization experiment permutation number.

7. The process of claim 1 wherein said predictive crystallization function analyzes a crystallization experimental sample as to a status selected from the group consisting of: clear drop, phase change, precipitate, and spherulettes.

8. The process of claim 1 wherein said predictive crystallization function trains through back propagation.

9. The process of claim 8 wherein said predictive crystallization function includes a hidden layer intermediate between input values and said optimal physical crystallization parameter.

10. The process of claim 1 wherein the performance of said plurality of crystallization experimental samples is automated.

11. The process of claim 10 further comprising the step of communicating said plurality of physical crystallization input variables between a manufacturing execution system performing said plurality of experimental samples and said predictive crystallization function.

12. The process of claim 1 further comprising the step of communicating said predictive crystallization function to a database.

13. The process of claim 12 wherein said database includes characteristics of a crystallization sample.

14. The process of claim 1 further comprising the steps of attempting crystal growth using said optimal physical crystallization parameter.

15. The process of claim 14 further comprising the step of communicating on said crystal growth attempt to a shared database.

16. The process of claim 15 further comprising the step of classifying said crystal growth attempt on a basis selected from the group consisting of: said optimal physical crystallization parameter, said predictive crystallization function, and a physical property of a crystallant.

17. The process of claim 1 wherein performing said plurality of crystallization experimental samples comprises the steps of:

controlling a plurality of variables where each of said plurality of variables assumes an index value or plurality of index values; and

performing a Chernov analysis to derive a minimized combined quantity representative of said total crystallization permutation number.

18. The process of claim 1 wherein said plurality of crystallization experimental samples are converted to vectors prior to the training of said predictive crystallization function.

19. The process of claim 18 further comprising the step of clustering said vectors.

20. The process of claim 19 wherein clustering occurs through the application of an analysis selected from the group consisting of: a neural net, a Chernov algorithm, a Bayesian net, a Bayesian classification schema, and a Bayesian decomposition.

21. A crystallization parameter optimization process comprising the steps of:

selecting a plurality of physical characterization input variables for a known crystallant to define a total crystallization experiment permutation number;

performing a plurality of crystallization experimental samples on said known crystallant;

training a predictive crystallization function through analysis of said plurality of crystallization experimental samples;

determining an optimal physical crystallization parameter for said known crystallant;

storing said optimal physical crystallization parameters and a physical property of said known crystallant sample in a classification system; and

comparing an unknown crystallization sample to the classification of said known crystallant.

22. The process of claim 21 wherein said predictive crystallization function is a neural network.

23. The process of claim 21 wherein said classification system is based on an aspect selected from the group consisting of: nodal basis functions, nodal construction similarities, and contribution of a particular physical characterization input variable.

24. The process of claim 21 wherein a comparative neural network relates said known crystallant and said unknown crystallization sample.

25. The process of claim 21 wherein said classification system is self-learning.

26. The process of claim 21 wherein said classification system is self-organized.

27. The process of claim 21 wherein each of said plurality of physical crystallization input variables is selected from a group consisting of: temperature, protein dilution, anionic precipitate, organic precipitate, buffer pH, precipitation strength, organic moment, percent glycerol, additive, divalent ion, gravity, light, magnetism, atmosphere identity, and atmosphere pressure.

28. The process of claim 21 wherein the performance of said plurality of crystallization experiments is automated.

29. The process of claim 21 further comprising the steps of attempting crystal growth using said optimal physical crystallization parameter.

30. The process of claim 21 wherein performing said plurality of crystallization experimental samples comprises the steps of:

controlling a plurality of variables where each of said plurality of variables assumes an index value or plurality of index values; and

performing a Chernov analysis to derive a minimized combined quantity representative of said total crystallization permutation number.

31. The process of claim 21 wherein storage occurs in a shared database wherein said shared database also stores at least one type of protein information selected from the group consisting of: protein expression gene; protein characteristics; protein class hierarchy; actual protein chemical structure including primary, secondary, tertiary and where applicable quaternary structures; protein crystal generation recipe parameters; and optimal crystallization screen design.

32. A protein crystal derived by the process of claim 1.

33. A neural network having been trained through analysis of a plurality of crystallization experimental samples to predict optimal crystallization conditions for a protein.

34. The network of claim 33 wherein said plurality of samples comprises samples failing to yield crystals.

35. A system for crystallization parameter optimization, the system comprising:

a database having a plurality of input variables, each of said plurality of input variables having a value range;

an incomplete factorial screen program having a trainable predictive crystallization function;

a computer capable of executing the incomplete factorial screen program to determine an optimal crystallization parameter; and

a manufacturing execution system for automatically acquiring of a datum from each of a plurality of crystallization experimental samples, analyzing and archiving of data from the incomplete factorial screen program.

36. The system of claim 35 wherein said manufacturing execution system controls at least one piece of crystallization hardware selected from the group consisting of: a liquid dispenser, a crystallant dispenser, a robotic handler, an imaging system, a sample centering motor relative to a camera focal plane, and a lighting system.

37. The system of claim 36 wherein said sample centering motor is coupled to at least one of: a sample stage and said camera for automatically positioning the specimen within the focal plane of said camera.

38. The system of claim 35 further comprising a barcode for indexing each of said plurality of samples.

39. The system of claim 36 further comprising a centering algorithm coupled to said motor for converging a central region of the specimen with a central region of the camera focal plane.

40. The system of claim 39 wherein said centering algorithm operates automatically.

41. The system of claim 35 further comprising a drop identification algorithm for evaluating a liquid drop associated with each of said plurality of samples.

42. The system of claim 41 wherein the liquid drop is classified into a preselected plurality of classes.

43. The system of claim 42 wherein said drop identification algorithm operates automatically.

44. The system of claim 36 wherein said motor is coupled to said camera.

45. The system of claim 36 further comprising scheduling software interfaced with said robotic handler.

46. The system of claim 37 wherein said scheduling software is interfaced with said sample stage.

47. The system of claim 35 further comprising a database that stores crystal relevant parameters.

48. The system of claim 47 wherein said crystal relevant parameters include at least one parameter of the group consisting of: crystal weight, crystal specimen pH, crystal specimen temperature, crystal specimen protein type, detergents present, additives present, preservatives present, reservoir buffer present, reservoir buffer concentration, reservoir buffer pH, crystal specimen volume, notes, crystal specimen score, and crystal specimen drop descriptor.

49. The system of claim 47 wherein said database is relational between said predictive crystallization function and said crystal parameters.

50. The system of claim 47 wherein said database is connected to a structured query language database.

51. A protein crystal derived from a system of claim 35.

52. A process according to claim 1 substantially as described herein in any of the examples.